Density Matrix of a Bose–Einstein Condensate: Steady–State versus Mean–Field Approach

S. J. Wang[1], M. C. Nemes[2], A. N. Salgueiro[3], and H. A. Weidenmüller[4]
[1] *Department of Modern Physics, University of Lanzhou, 730000 Lanzhou, P.R. China*
[2] *Department of Physics, University of Belo Horizonte, Belo Horizonte, Minas Gerais, Brasil*
[3] *Max-Planck-Institut für Physik komplexer Systeme , D-01187 Dresden, Germany*
[4] *Max-Planck-Institut für Kernphysik, D-69029 Heidelberg, Germany*
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We compare the equilibrium solution for the condensate obtained in the mean–field approximation to the master equation for sympathetic cooling with the one obtained by Scully for a system in contact with a heat bath with the help of an analogy with the laser. While the mean–field approach yields analytical formulas for the approach towards equilibrium and for the equilibrium solution, it neglects the correlations between occupation numbers of different single–particle states which are approximately kept in Scully's approach. Such neglect is admissible as long as the fraction of Bosons in the condensate does not exceed a few percent or so.

Motivation. The experimental realization of Bose–Einstein condensation [1] calls for a thorough theoretical understanding of the properties of the condensate. An important step in this direction was recently taken by Scully *et al.* [2,3]. Using the analogy between the condensate and a laser, these authors derived the equilibrium form of the reduced density matrix ρ_0 of the condensate for a system containing a fixed number N_A of Bosons. The result is obtained as the steady–state solution of the time–dependent non–equilibrium master equation for an ideal Bose gas in a three–dimensional harmonic trap coupled to a thermal reservoir. The particle number N_A serves as an important constraint. The solution found in Refs. [2,3] has the form

$$\rho_0 = \sum_{N \le N_A} \frac{1}{Z_{N_A}} \left[N_A (\frac{T}{T_c})^3 \right]^{N_A - N} \Pi^N \ . \tag{1}$$

Here $\Pi^N = |N\rangle_0 \ {}_0\langle N|$ is the projector onto the lowest single–particle state containing $N \le N_A$ Bosons. The temperature of the reservoir is denoted by T, while T_c is a suitably defined transition temperature, and Z_N is a normalization factor.

Another starting point towards understanding the properties of the condensate is the master equation for sympathetic cooling. This master equation was, in very general form, derived in Ref. [4]. The cooling agent is a cooled gas in thermal equilibrium. The cooling mechanisms for a system in contact with a reservoir [2] and for a system subject to sympathetic cooling [4] differ. In the first case, energy is exchanged via exciting or de–exciting the reservoir. In the second case, cooling is due to two–body collisions between the atoms in the cooling gas and those in the system of N_A Bosons. The form given in Eq. (1) for the density matrix of the condensate is also obtained from the master equation for sympathetic cooling [5] by postulating that the elements of the density matrix referring to excited single–particle states have attained the equilibrium form but that this form depends on the number N of Bosons in the ground–state configuration $|N\rangle_0$. The agreement between the forms of ρ_0 found from two different approaches gives confidence that Eq. (1) represents a good approximation to the true from of the density matrix for the condensate.

Recently, the present authors have developed a mean–field approach to the master equation for sympathetic cooling [6]. This approach yields explicit analytic expressions for the density matrix of both, the condensate and the N_A–Boson system in excited single–particle states. The approach yields not only the equilibrium solution but also the time–dependence of the cooling process. The reason is that the mean–field equations possess a $SU(1,1)$ dynamical symmetry. Therefore, the equations are integrable [7,8].

In the present Letter, we compare the equilibrium solution for the density matrix ρ_0 of the condensate as obtained from the mean–field approximation with Eq. (1). The comparison will cast new light on both, the form of ρ_0 and the limitation of the mean–field approach. In addition, we briefly display the time evolution towards equilibrium as obtained in the mean–field approach.

Master Equation. Starting point is the master equation derived in Ref. [4]. We use the notation of Refs. [4,5]. We label the system subject to sympathetic cooling as system A. This system consists of N_A Bosons. The master equation for the dependence of the reduced density matrix $\rho_A(t)$ for system A on time t reads

$$\frac{\mathrm{d}\rho_A(t)}{\mathrm{d}t} = -\frac{i}{\hbar}\left[H_A + H'_{A-A}, \rho_A(t) \right] + \mathcal{L}\rho_A \ . \tag{2}$$

Here, H_A is the sum of the single–particle Hamiltonians for the atoms in system A (each containing the kinetic energy and the harmonic trap potential) while H'_{A-A} represents the (weak) interaction between the atoms in system A. This interaction is neglected in what follows because sympathetic cooling is used precisely when H'_{A-A} is very

small. The action of the Liouvillean $\mathcal{L}$ on the reduced density matrix $\rho_A(t)$ is given by

$$\mathcal{L}\rho_A = \sum_{\vec{n},\vec{n}',\vec{m},\vec{m}'} \Gamma^{\vec{m},\vec{m}'}_{\vec{n},\vec{n}'} \Big(2a^\dagger_{\vec{m}} a_{\vec{m}'} \rho_A(t) a^\dagger_{\vec{n}} a_{\vec{n}'} - a^\dagger_{\vec{n}} a_{\vec{n}'} a^\dagger_{\vec{m}} a_{\vec{m}'} \rho_A(t) - \rho_A(t) a^\dagger_{\vec{n}} a_{\vec{n}'} a^\dagger_{\vec{m}} a_{\vec{m}'} \Big) . \quad (3)$$

The single–particle states of the three–dimensional isotropic harmonic trap are labelled by the quantum numbers $\vec{m} = (m_x, m_y, m_z)$ with m_x, m_y, m_z integer. The creation and annihilation operators for these states are written as $a^\dagger_{\vec{m}}$ and $a_{\vec{m}}$, respectively. The index 0 is used for the non–degenerate ground state of the trap. The rate coefficients $\Gamma^{\vec{m},\vec{m}'}_{\vec{n},\vec{n}'}$ are given in Ref. [4]. We do not repeat the definition here. Suffice it to say that these coefficients account for the interaction between particles in system A and those in the cooling system B. We assume that the number N_B of atoms in system B is very large. Then decoherence acts very quickly [5] and reduces the density matrix to diagonal form. Hence,

$$\mathcal{L}\rho_A = \sum_{\vec{m}\neq\vec{n}} \Gamma^{\vec{m},\vec{n}}_{\vec{n},\vec{m}} \Big(2a^\dagger_{\vec{m}} a_{\vec{n}} \rho_A(t) a^\dagger_{\vec{n}} a_{\vec{m}} - a^\dagger_{\vec{n}} a_{\vec{m}} a^\dagger_{\vec{m}} a_{\vec{n}} \rho_A(t) - \rho_A(t) a^\dagger_{\vec{n}} a_{\vec{m}} a^\dagger_{\vec{m}} a_{\vec{n}} \Big) . \quad (4)$$

Mean–Field Approximation. Eq. (4) serves as the starting point for the mean–field approximation. We apply this approximation in standard fashion by replacing on the right–hand side of Eq. (4) one pair of creation and annihilation operators referring to the same single–particle state $\vec{m}$ or $\vec{n}$ by its expectation value $\langle a^\dagger_{\vec{m}} a_{\vec{m}} \rangle$. The quantity

$$N_{\vec{m}} = \langle a^\dagger_{\vec{m}} a_{\vec{m}} \rangle = \mathrm{tr}(a^\dagger_{\vec{m}} a_{\vec{m}} \rho_A) \quad (5)$$

is the mean particle occupation number of the single–particle state $\vec{m}$. For the term $\mathcal{L}\rho_A$, this procedure yields

$$\begin{aligned} \mathcal{L}\rho_A = & \sum_{\vec{m}\neq\vec{n}} \Gamma^{\vec{m},\vec{n}}_{\vec{n},\vec{m}} \; N_{\vec{n}} \; \Big(2a^\dagger_{\vec{m}} \rho_A(t) a_{\vec{m}} - a^\dagger_{\vec{m}} a_{\vec{m}} \rho_A(t) - \rho_A(t) a_{\vec{m}} a^\dagger_{\vec{m}} - \rho_A \Big) \\ & + \sum_{\vec{m}} \Gamma^{\vec{n}\vec{m}}_{\vec{m}\vec{n}} \; (N_{\vec{n}} + 1) \; \Big(2a_{\vec{m}} \rho_A(t) a^\dagger_{\vec{m}} - a^\dagger_{\vec{m}} a_{\vec{m}} \rho_A(t) - \rho_A(t) a_{\vec{m}} a^\dagger_{\vec{m}} + \rho_A \Big) . \end{aligned} \quad (6)$$

Central to the mean–field approach is the assumption that there are no correlations between the occupation probabilities of the harmonic trap levels $\vec{n}$ and $\vec{m}$.

Rate Equation. Eqs. (2) and (6) can be reduced to a rate equation. We use a basis in Hilbert space defined by a product of all single–particle states $\vec{m}$, each such state being occupied by $N_{\vec{m}}$ Bosons. We take the trace of $\rho_A(t)$ over all single–particle states $\vec{n}$ with $\vec{n} \neq \vec{m}$ (this includes a summation over all occupation numbers $N_{\vec{m}}$) and denote the result by $\rho_{\vec{m}}(t)$. That same notation was used already in Eq. (1) with $\vec{m} = 0$. We recall that $\rho_A(t)$ is diagonal in energy representation. It follows that $\rho_{\vec{m}}(t)$ can be written as a sum of the projectors $\Pi^N_{\vec{m}} = |N\rangle_{\vec{m}\,\vec{m}}\langle N|$,

$$\rho_{\vec{m}}(t) = \sum_{N=0}^{N_A} P^N_{\vec{m}}(t) \; \Pi^N_{\vec{m}} . \quad (7)$$

The time–dependent mean–field occupation probabilities $P^N_{\vec{m}}(t)$ differ from zero only for $N \leq N_A$. Taking the corresponding trace of Eq. (2) and using Eq. (6), we find that the $P^N_{\vec{m}}(t)$ obey the rate equation

$$\begin{aligned} \frac{\mathrm{d}P^N_{\vec{m}}(t)}{\mathrm{d}t} = & \, 2K_{\vec{m}} N P^{N-1}_{\vec{m}} + 2H_{\vec{m}}(N+1) P^{N+1}_{\vec{m}} \\ & - 2(K_{\vec{m}} + H_{\vec{m}}) N P^N_{\vec{m}} - 2K_{\vec{m}} P^N_{\vec{m}} . \end{aligned} \quad (8)$$

The cooling and heating coefficients K_m and H_m are given by

$$\begin{aligned} K_{\vec{m}} &= \sum_{\vec{n}\neq\vec{m}} \Gamma^{\vec{m},\vec{n}}_{\vec{n},\vec{m}} N_{\vec{n}} , \\ H_{\vec{m}} &= \sum_{\vec{n}\neq\vec{m}} \Gamma^{\vec{n},\vec{m}}_{\vec{m},\vec{n}} (N_{\vec{n}} + 1) . \end{aligned} \quad (9)$$

¿From Eqs. (5,7) and (8) we obtain for the mean occupation number $N_{\vec{m}}(t)$

$$\frac{\mathrm{d}N_{\vec{m}}}{\mathrm{d}t} = 2K_{\vec{m}} \; (N_{\vec{m}} + 1) - 2H_{\vec{m}} \; N_{\vec{m}} . \quad (10)$$

This equation is consistent with conservation of particle number, $\sum_{\vec{m}} \mathrm{d}N_{\vec{m}}/\mathrm{d}t = 0$.

Condensate. Putting $\vec{m} = 0$ in Eq. (8), one obtains the equation for the probability distribution of the number of atoms in the single–particle ground state, i.e., the condensate. The equilibrium solution obeys $\mathrm{d}P^N_0(t)/\mathrm{d}t = 0$. It is easily seen that the resulting equations for the time–independent coefficients P^N_0 do not possess a non–trivial solution. This is because the constraint $P^N_0 = 0$ for $N > N_A$ is too rigid for the mean–field approach. We relax this condition, write

$$\rho_0(t) = \sum_{N=0}^{\infty} P^N_0(t) \; \Pi^N_{\vec{m}} \quad (11)$$

and require only that the sum $\sum_{N=N_A}^{\infty} P^N_0$ be negligibly small. The resulting equation for the P^N_0's reads

$$\begin{aligned} & 2K_0 N P^{N-1}_0 + 2H_0(N+1) P^{N+1}_0 - 2(H_0 + K_0) N P^N_0 \\ & - 2K_0 P^N_0 = 0 , \qquad N = 0, \ldots, \infty . \end{aligned} \quad (12)$$

The solution is

$$P_0^N = P_0^0\ \chi^N \quad \text{where} \quad \chi = \frac{K_0}{H_0}\ . \tag{13}$$

Eq. (10) implies that in the stationary case we must have $\chi < 1$. The normalization condition yields $P_0^0 = (1-\chi)$. The mean value N_0 is given by $N_0 = \chi/(1-\chi)$. Conversely, we may replace χ everywhere by $N_0/(N_0+1)$. To discuss the validity of the mean–field solution, we impose the constraint that $\sum_{N=N_A}^{\infty} P_0^N/P_0^0 = \chi^{N_A}/(1-\chi) < \exp(-a)$. For $N_A \gg 1$, this yields $N_0/N_A < 1/a$. This condition applies as long as $a \gg \ln(N_0)$ and shows that for the condensate, the mean–field approximation (as defined in the framework of this paper) begins to fail whenever the ratio N_0/N_A grows beyond a few percent or so. Similar conclusions apply to the stationary occupation probabilities $P_{\vec{m}}^N$ of excited single–particle states, except that here we do not expect the mean occupation number ever to approach values close to N_A.

The $P_0^N \sim \chi^N$ given by Eq. (13) decrease monotonically with increasing N. This behavior is in marked contrast to that of the equilibrium solution Eq. (1) found first by Scully [2,3] and reproduced, in the present context, in Ref. [5]. The ground–state distribution as given by Eq. (1) is Poissonian, except for the additional normalization factor.

The physical situations encapsulated in Eqs. (1) and (13) are completely analogous to the behavior of a laser far above and below threshold, respectively [9]. The difference between Eqs. (1) and (13) is due to the strong correlations between the numbers of particles in excited single–particle states and in the ground state. That correlation is taken into account approximately in the derivation of Eq. (1). Indeed, in this derivation it is assumed that for $\vec{m} \neq 0$ we have $\langle a^{\dagger}_{\vec{m}} a_{\vec{m}} \rangle = N_{\vec{m}}(N)$ with $N_{\vec{m}}(N)$ constrained by N, the number of Bosons in the ground–state configuration $|N\rangle_0$. The resulting nonlinearity is analogous to the nonlinearity which governs the behavior of a laser far above threshold. It carries the solution beyond the mean–field approximation and is well suited to describe the probability distribution of the atoms in the condensate whenever their number is of the order of N_A. As mentioned in the beginning, there is good reason to believe that Eq. (1) correctly describes this situation. In the mean–field approach, on the other hand, the correlations between the numbers of particles in the excited single–particle states and in the ground state are totally neglected. This situation is analogous to the behavior of a laser below threshold (linear case). We conclude that Eqs. (1) and (13) describe two different regimes. The equilibrium solution Eq. (13) describes a system where at most a few percent of the atoms are in the ground state. As that fraction increases, there is a gradual transition to another regime described by Eq. (1). The intermittent case is apparently not covered by either formula.

In the remainder of the paper, we demonstrate that the mean–field approximation is well suited to describe the approach of the system towards equilibrium, and not only the stationary case. This is due to the fact that the master equation is linear in the generators of the group $SU(1,1)$. Details of the calculation are given elsewhere [6]. Writing the time–dependent master equation in the form

$$\frac{\mathrm{d}\rho_{\vec{m}}(t)}{\mathrm{d}t} = \Gamma(t)\rho_{\vec{m}}(t)\ , \tag{14}$$

with $\Gamma(t)$ dependent upon time, we construct a time–dependent similarity transformation $T(t)$ which diagonalizes $\Gamma(t)$. Because of the form of Γ, there exist two different similarity transformations which accomplish this aim. However, only one of the two fulfills the condition for the viability of the mean–field solution, namely, that the coefficients multiplying Π^N vanish asymptotically for large N. Using this transformation, the time–evolution of the reduced density matrix can be determined and is given by

$$\begin{aligned} \rho_{\vec{m}}(t) &= \exp[\alpha_+(t)K^+]\ \exp[\alpha_-(t)K^-] \\ &\times \exp\left(\int_0^t \mathrm{d}\tau[\gamma(\tau)K^0 - K_m(\tau) - H_m(\tau))]\right)\ \rho_{\vec{m}}(0) \end{aligned} \tag{15}$$

where $\rho_{\vec{m}}(0)$ is fixed by the initial condition, and $\gamma(t) = 4H_m(t)\alpha_+(t) - 2[K_m(t) + H_m(t)]$. The time–dependent functions $\alpha_{\pm}(t)$ are the solutions of the differential equations

$$\begin{aligned} \frac{\mathrm{d}\alpha_+(t)}{\mathrm{d}t} &= 2K_m + 2H_m\alpha_+^2 - 2(K_m + H_m)\ \alpha_+ \\ \frac{\mathrm{d}\alpha_-(t)}{\mathrm{d}t} &= 2H_m\ (1 - 2\alpha_+\alpha_-) + 2(K_m + H_m)\ \alpha_-\ . \end{aligned} \tag{16}$$

The initial conditions are $\alpha_{\pm}(0) = 0$. The action of the operators K^+, K^- and K^0 on the quantities $\Pi_{\vec{m}}^{n,k} = |n\rangle_{\vec{m}\vec{m}}\langle k|$ is given by

$$\begin{aligned} K^0_{\vec{m}}\Pi_{\vec{m}}^{n,k} &= \frac{1}{2}(n+k+1)\Pi_{\vec{m}}^{n,k}\ , \\ K^+_{\vec{m}}\Pi_{\vec{m}}^{n,k} &= \sqrt{(n+1)(k+1)}\ \Pi_{\vec{m}}^{n+1,k+1}\ , \\ K^-_{\vec{m}}\Pi_{\vec{m}}^{n,k} &= \sqrt{nk}\ \Pi_{\vec{m}}^{n-1,k-1}\ . \end{aligned} \tag{17}$$

¿From the asymptotic behavior of the coefficients K_m, H_m, γ and $\alpha_{\pm}$, it can be shown that as $t \to \infty$, $\rho_{\vec{m}}(t)$ approaches the equilibrium solution which for $\vec{m} = 0$ is displayed in Eq. (13).

In summary, our results show that the mean–field approach is a useful tool to investigate both sympathetic cooling and properties of the condensate. The limiting factor in the approach is the neglect of correlations between occupation numbers in the ground state and in excited single–particle states. Such correlations generate a non-linear term in the cooling and heating coefficients

and become important whenever the fraction of Bosons in the condensate exceeds a few percent or so. While the master equation for the mean–field approach allows for an analytical solution, it is unlikely that such a solution exists in the general case. The distributions of occupation probabilities of states with N_0 Bosons in the ground state differ very much in the mean–field approach and in the approximation obtained by Scully. The latter is probably adequate whenever the fraction of Bosons in the ground state is of order unity. The two distributions display similarities with the behavior of a laser below and far above threshold, respectively.

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